

distributed among said dummy atoms and wherein said center atom has a charge of zero.

38. (amended) The computer readable medium of claim 37 wherein said dummy atom has a mass of about 0.1 g/mol.
39. (amended) The computer readable medium of claim 37 wherein said dummy atom has a mass greater than about 0.1 g/mol.
40. (amended) The computer readable medium of claim 37 wherein said dummy atoms are located at the apices of a polyhedron.
41. (amended) The computer readable medium of claim 40 wherein said center atom is located at the center of said polyhedron.
42. (amended) The computer readable medium of claim 40 wherein said polyhedron is selected from the group consisting of trigonal, tetrahedron, pentahedron, hexagonal, septagonal, and octahedral.
43. (amended) The computer readable medium of claim 41 wherein said polyhedron is a tetrahedron.
44. (amended) The computer readable medium of claim 37 wherein said metal ion is selected from a main group metal or transition metal.
45. (amended) The computer readable medium of claim 37 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.

46. (amended) The computer readable medium of claim 37 wherein said metal ion is zinc.
47. (amended) The computer readable medium of claim 41 wherein said metal ion is zinc.
48. (amended) The computer readable medium of claim 37 wherein said metal ion is magnesium.
49. (amended) The computer readable medium of claim 37 wherein said metal ion is calcium.
50. (amended) The computer readable medium of claim 37 wherein said metal ion has a calculated energy of solvation about equal to an experimentally determined energy of solvation for said metal ion.
51. (amended) The computer readable medium of claim 50 wherein said calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.
52. (amended) The computer readable medium of claim 37 wherein said dummy atom has a charge of about 0.5.
53. (amended) The computer readable medium of claim 37 wherein said dummy atom has a charge of about 0.3333.
54. (amended) The computer readable medium of claim 37 wherein said dummy atom has a charge ranging from about +0.1 to about +3.

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55. (new) A computer readable medium having computer executable instructions stored thereon, that when executed simulate a metal ion for use in a molecular dynamics simulation comprising a center atom having a van der Waals radius greater than zero covalently linked to one or more dummy atoms having a van der Waals radius of about zero, wherein the overall charge of said metal ion is evenly distributed among said dummy atoms and wherein said center atom has a charge of zero.
56. (new) The computer readable medium of claim 55 wherein said dummy atom has a mass of about 0.1 g/mol.
57. (new) The computer readable medium of claim 55 wherein said dummy atom has a mass greater than about 0.1 g/mol.
58. (new) The computer readable medium of claim 55 wherein said dummy atoms are located at the apices of a polyhedron.
59. (new) The computer readable medium of claim 58 wherein said center atom is located at the center of said polyhedron.
60. (new) The computer readable medium of claim 58 wherein said polyhedron is selected from the group consisting of trigonal, tetrahedron, pentahedron, hexagonal, septagonal, and octahedral.
61. (new) The computer readable medium of claim 59 wherein said polyhedron is a tetrahedron.
62. (new) The computer readable medium of claim 55 wherein said metal ion is selected from a main group metal or transition metal.

63. (new) The computer readable medium of claim 55 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.
64. (new) The computer readable medium of claim 55 wherein said metal ion is zinc.
65. (new) The computer readable medium of claim 59 wherein said metal ion is zinc.
66. (new) The computer readable medium of claim 55 wherein said metal ion is magnesium.
67. (new) The computer readable medium of claim 55 wherein said metal ion is calcium.
68. (new) The computer readable medium of claim 55 wherein said metal ion has a calculated energy of solvation about equal to an experimentally determined energy of solvation for said metal ion.
69. (new) The computer readable medium of claim 68 wherein said calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.
70. (new) The computer readable medium of claim 55 wherein said dummy atom has a charge of about 0.5.
71. (new) The computer readable medium of claim 55 wherein said dummy atom has a charge of about 0.3333.
72. (new) The computer readable medium of claim 55 wherein said dummy atom has a charge ranging from about +0.1 to about +3.